



DETERMINATION OF THE CONCENTRATIONS OF THE REACTANTS OF FIRST ORDER CONSECUTIVE CHEMICAL REACTION USING ANUJ TRANSFORM

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ABSTRACT: The study of chemical reactions plays the vital role for understanding the problems of science and engineering such as photosynthesis; heat mass transfer; nuclear reactor; photon emission and radioactive decay. The main objective of this manuscript is to make use of Anuj transform in order to analytically determine the solution of the problem of concentrations of the reactants of first order consecutive chemical reaction. Results suggested that Anuj transform is efficient method for determining the solution of the problem of concentrations of the reactants of first order consecutive chemical reaction. Results of the manuscript demonstrate that Anuj transform has good accuracy and provide exact results without doing intricate calculation work.

KEYWORDS: Anuj Transform; Inverse Anuj Transform; Cramer Rule; Chemical Reaction; Concentration; Reactant.

MATHEMATICS SUBJECT CLASSIFICATION: 35A22; 44A05; 34A30; 65L05; 80A30

1.INTRODUCTION: In the recent years, integral transforms are the first preference of the researchers for tackling the problem of growth of the species [1-12]; decay problem of radioactive substance [1-10]; Abel's problem of mechanics [13-20]; heat problem [21]; circuit problems of electronics communication [22]; problem of infected cells during infection of HIV-1 [23]; concentration problem of drug during intravenous injection of drug [24-25] and vibration problem of string [21-22] because integral transforms provide the exact primitives of these problems. Researchers are also very interested for developing new integral transforms [26-27] nowadays due to their high-yielding characteristic of providing results of the problems with good accuracy.

Researchers [28-35] developed the duality relation among the different integral transforms and successfully utilized these relations for developing new properties and theories of integral transforms. Higazy and Aggarwal [36] applied Sawi transform on the mathematical model of the chemical reaction in series and estimated the concentration of chemical substances. Murphy [37] analyzed the consecutive chemical reactions of first and second orders. Lin [38] analyzed the consecutive reactions (homogeneous) performed in an annular reactor with non Newtonian flow.

Chrastil [39] obtained the value of rate constants of consecutive chemical reaction of first order by the aid of final product. The mathematical models of the consecutive reactions were suggested by Westman and DeLury [40]. Erdogdn and Sahmurat [41] obtained the kinetic constants of first-order consecutive chemical reactions. The main interest of this manuscript is to determine the solution of the problem of concentrations of the reactants of first order consecutive chemical reaction via Anuj transform. This study has a great practical importance due to achieve maximum production by eliminating waste or useless products in the transitional phase of chemical reaction.

2. NOMENCLATURE OF SYMBOLS

\mathcal{F} , family of piecewise continuous and exponential order function;

\mathcal{A} , Anuj transform operator;

\mathcal{A}^{-1} , inverse Anuj transform operator;

\in , belongs to;

!, the usual factorial notation;

Γ , the classical Gamma function;

\mathcal{L} , Laplace transform operator;

N , the set of natural numbers;

R , the set of reals;

$\theta_1(t)$, concentration of a chemical reactant P at any time t ;

$\theta_2(t)$, concentration of a chemical reactant Q at any time t ;

$\theta_3(t)$, concentration of a chemical reactant R at any time t ;

$\theta_1(0) = \omega$, initial concentration of a chemical reactant P ;

$\theta_2(0)$, initial concentration of a chemical reactant Q ;

$\theta_3(0)$, initial concentration of a chemical reactant R ;

$\beta_1, \beta_2 > 0$, rate constants

3. DEFINITION OF ANUJ TRANSFORM

If $H(t) \in \mathcal{F}, t \geq 0$ then the Anuj transform of $H(t)$ is defined as [26]

$$\mathcal{A}\{H(t)\} = r^2 \int_0^\infty H(t)e^{-\left(\frac{1}{r}\right)t} dt = h(r), \quad r > 0 \quad (1)$$

4. INVERSE ANUJ TRANSFORM

The inverse Anuj transform of $h(r)$, denoted by $\mathcal{A}^{-1}\{h(r)\}$, is another function $H(t)$ having the characteristic that

$$\mathcal{A}\{H(t)\} = h(r).$$

5. RELATION BETWEEN LAPLACE AND ANUJ TRANSFORMS

$$\text{If } \mathcal{L}\{H(t)\} = \int_0^\infty H(t)e^{-rt} dt = \Psi(r), \quad (2)$$

$$\text{then } h(r) = r^2 \Psi\left(\frac{1}{r}\right) \quad (3)$$

$$\text{and } \Psi(r) = r^2 h\left(\frac{1}{r}\right) \quad (4)$$

Proof: Equation (1) gives

$$h(r) = r^2 \int_0^\infty H(t)e^{-\left(\frac{1}{r}\right)t} dt = r^2 \left\{ \int_0^\infty H(t)e^{-\left(\frac{1}{r}\right)t} dt \right\} = r^2 \Psi\left(\frac{1}{r}\right)$$

Now equation (2) gives

$$\Psi(r) = \int_0^\infty H(t)e^{-rt} dt = r^2 \left\{ \frac{1}{r^2} \int_0^\infty H(t)e^{-rt} dt \right\} = r^2 h\left(\frac{1}{r}\right).$$

6. PROPERTIES OF ANUJ TRANSFORM: In this part, we will describe the properties of Anuj transform that will be used in later section of this manuscript.

6.1 Linearity [24]: If $H_j(t) \in \mathcal{F}, t \geq 0, j = 1, 2, 3, \dots, n$ with $\mathcal{A}\{H_j(t)\} = h_j(r), j = 1, 2, 3, \dots, n$ then $\mathcal{A}\{\sum_{j=1}^n \ell_j H_j(t)\} = \sum_{j=1}^n \ell_j \mathcal{A}\{H_j(t)\} = \sum_{j=1}^n \ell_j h_j(r)$, where ℓ_j are arbitrary constants.

6.2 Change of Scale [24]: If $H(t) \in \mathcal{F}, t \geq 0$ with $\mathcal{A}\{H(t)\} = h(r)$ then $\mathcal{A}\{H(\ell t)\} = \frac{1}{\ell^3} h(\ell r)$, where ℓ is arbitrary constant.

6.3 Translation [24]: If $H(t) \in \mathcal{F}, t \geq 0$ with $\mathcal{A}\{H(t)\} = h(r)$ then

$$\mathcal{A}\{e^{\ell t} H(t)\} = (1 - \ell r)^2 h\left(\frac{r}{1 - \ell r}\right), \text{ where } \ell \text{ is arbitrary constant.}$$

Remark 1: Equations (3) and (4) can be use for establishing the further properties of Anuj transform.

7. ANUJ TRANSFORMS OF THE DERIVATIVES OF A FUNCTION [12]: If $H(t) \in \mathcal{F}, t \geq 0$ with $\mathcal{A}\{H(t)\} = h(r)$ then

$$\text{a) } \mathcal{A}\{H'(t)\} = \frac{1}{r} h(r) - r^2 H(0).$$

$$\text{b) } \mathcal{A}\{H''(t)\} = \frac{1}{r^2} h(r) - rH(0) - r^2 H'(0).$$

$$\text{c) } \mathcal{A}\{H'''(t)\} = \frac{1}{r^3} h(r) - H(0) - rH'(0) - r^2 H''(0).$$

Remark 2: Tables 1-2 visualized the Anuj transforms and inverse Anuj transforms of fundamental functions respectively.

Table-1: Anuj transforms of fundamental functions [26]

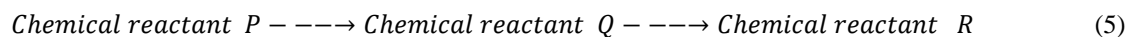
S.N.	$H(t) \in \mathcal{F}, t > 0$	$\mathcal{A}\{H(t)\} = h(r)$
1	1	r^3
2	$e^{\ell t}$	$\left(\frac{r^3}{1 - \ell r}\right)$
3	$t^\lambda, \lambda \in N$	$\lambda! r^{\lambda+3}$
4	$t^\lambda, \lambda > -1, \lambda \in R$	$r^{\lambda+3} \Gamma(\lambda + 1)$
5	$\sin(\ell t)$	$\left(\frac{\ell r^4}{1 + r^2 \ell^2}\right)$
6	$\cos(\ell t)$	$\left(\frac{r^3}{1 + r^2 \ell^2}\right)$
7	$\sinh(\ell t)$	$\left(\frac{\ell r^4}{1 - r^2 \ell^2}\right)$
8	$\cosh(\ell t)$	$\left(\frac{r^3}{1 - r^2 \ell^2}\right)$

Table-2: Inverse Anuj transforms of fundamental functions

S.N.	$h(r)$	$H(t) = \mathcal{A}^{-1}\{h(r)\}$
1	r^3	1
2	$\left(\frac{r^3}{1 - \ell r}\right)$	$e^{\ell t}$
3	$r^{\lambda+3}, \lambda \in N$	$\frac{t^\lambda}{\lambda!}$
4	$r^{\lambda+3}, \lambda > -1, \lambda \in R$	$\frac{t^\lambda}{\Gamma(\lambda + 1)}$
5	$\left(\frac{r^4}{1 + r^2 \ell^2}\right)$	$\frac{\sin(\ell t)}{\ell}$
6	$\left(\frac{r^3}{1 + r^2 \ell^2}\right)$	$\cos(\ell t)$
7	$\left(\frac{r^4}{1 - r^2 \ell^2}\right)$	$\frac{\sinh(\ell t)}{\ell}$
8	$\left(\frac{r^3}{1 - r^2 \ell^2}\right)$	$\cosh(\ell t)$

8. DETERMINATION OF THE CONCENTRATIONS OF THE REACTANTS OF FIRST ORDER CONSECUTIVE CHEMICAL REACTION USING ANUJ TRANSFORM:

The concentrations $\theta_1(t)$, $\theta_2(t)$ and $\theta_3(t)$ of three chemical reactants P , Q and R of first order consecutive chemical reaction



at any time t is determined by the following system of linear ordinary differential equations as [36]

$$\left. \begin{aligned} \frac{d\theta_1}{dt} &= -\beta_1\theta_1 \\ \frac{d\theta_2}{dt} &= \beta_1\theta_1 - \beta_2\theta_2 \\ \frac{d\theta_3}{dt} &= \beta_2\theta_2 \end{aligned} \right\} \quad (6)$$

with $\theta_1(0) = \omega$, $\theta_2(0) = 0$ and $\theta_3(0) = 0$ (7)

Performing Anuj transform on equation (6), we have

$$\left. \begin{aligned} \mathcal{A}\left\{\frac{d\theta_1}{dt}\right\} &= -\mathcal{A}\{\beta_1\theta_1\} \\ \mathcal{A}\left\{\frac{d\theta_2}{dt}\right\} &= \mathcal{A}\{\beta_1\theta_1 - \beta_2\theta_2\} \\ \mathcal{A}\left\{\frac{d\theta_3}{dt}\right\} &= \mathcal{A}\{\beta_2\theta_2\} \end{aligned} \right\} \quad (8)$$

Use of 6.1 in equation (8) gives

$$\left. \begin{aligned} \mathcal{A}\left\{\frac{d\theta_1}{dt}\right\} &= -\beta_1\mathcal{A}\{\theta_1\} \\ \mathcal{A}\left\{\frac{d\theta_2}{dt}\right\} &= \beta_1\mathcal{A}\{\theta_1\} - \beta_2\mathcal{A}\{\theta_2\} \\ \mathcal{A}\left\{\frac{d\theta_3}{dt}\right\} &= \beta_2\mathcal{A}\{\theta_2\} \end{aligned} \right\} \quad (9)$$

Use of 7 (a) in equation (9) gives

$$\left. \begin{aligned} \frac{1}{r}\mathcal{A}\{\theta_1\} - r^2\theta_1(0) &= -\beta_1\mathcal{A}\{\theta_1\} \\ \frac{1}{r}\mathcal{A}\{\theta_2\} - r^2\theta_2(0) &= \beta_1\mathcal{A}\{\theta_1\} - \beta_2\mathcal{A}\{\theta_2\} \\ \frac{1}{r}\mathcal{A}\{\theta_3\} - r^2\theta_3(0) &= \beta_2\mathcal{A}\{\theta_2\} \\ \left. \begin{aligned} \left(\frac{1}{r} + \beta_1\right)\mathcal{A}\{\theta_1\} - r^2\theta_1(0) &= 0 \\ \Rightarrow -\beta_1\mathcal{A}\{\theta_1\} + \left(\frac{1}{r} + \beta_2\right)\mathcal{A}\{\theta_2\} - r^2\theta_2(0) &= 0 \\ \beta_2\mathcal{A}\{\theta_2\} + \frac{1}{r}\mathcal{A}\{\theta_3\} - r^2\theta_3(0) &= 0 \end{aligned} \right\} \end{aligned} \right\} \quad (10)$$

Use of equation (7) in equation (10) provides

$$\left. \begin{aligned} \left(\frac{1}{r} + \beta_1\right)\mathcal{A}\{\theta_1\} - r^2\omega &= 0 \\ -\beta_1\mathcal{A}\{\theta_1\} + \left(\frac{1}{r} + \beta_2\right)\mathcal{A}\{\theta_2\} &= 0 \\ \beta_2\mathcal{A}\{\theta_2\} + \frac{1}{r}\mathcal{A}\{\theta_3\} &= 0 \\ \left. \begin{aligned} \left(\frac{1}{r} + \beta_1\right)\mathcal{A}\{\theta_1\} &= r^2\omega \\ \Rightarrow -\beta_1\mathcal{A}\{\theta_1\} + \left(\frac{1}{r} + \beta_2\right)\mathcal{A}\{\theta_2\} &= 0 \\ \beta_2\mathcal{A}\{\theta_2\} + \frac{1}{r}\mathcal{A}\{\theta_3\} &= 0 \end{aligned} \right\} \end{aligned} \right\} \quad (11)$$

Equation (11) represents a system of three non-homogeneous linear equations in $\mathcal{A}\{\theta_1\}$, $\mathcal{A}\{\theta_2\}$ and $\mathcal{A}\{\theta_3\}$ unknowns. Now use of Cramer's rule in equation (11) gives the values of unknowns $\mathcal{A}\{\theta_1\}$, $\mathcal{A}\{\theta_2\}$ and $\mathcal{A}\{\theta_3\}$ as:

$$\mathcal{A}\{\theta_1\} = \frac{\begin{vmatrix} r^2\omega & 0 & 0 \\ 0 & \left(\frac{1}{r} + \beta_2\right) & 0 \\ 0 & \beta_2 & \frac{1}{r} \end{vmatrix}}{\begin{vmatrix} \left(\frac{1}{r} + \beta_1\right) & 0 & 0 \\ -\beta_1 & \left(\frac{1}{r} + \beta_2\right) & 0 \\ 0 & \beta_2 & \frac{1}{r} \end{vmatrix}}, \quad \begin{vmatrix} \left(\frac{1}{r} + \beta_1\right) & 0 & 0 \\ -\beta_1 & \left(\frac{1}{r} + \beta_2\right) & 0 \\ 0 & \beta_2 & \frac{1}{r} \end{vmatrix} \neq 0$$

$$\Rightarrow \mathcal{A}\{\theta_1\} = \left(\frac{\omega r^3}{1+\beta_1 r}\right) \quad (12)$$

$$\mathcal{A}\{\theta_2\} = \frac{\begin{vmatrix} \left(\frac{1}{r} + \beta_1\right) & r^2\omega & 0 \\ -\beta_1 & 0 & 0 \\ 0 & 0 & \frac{1}{r} \end{vmatrix}}{\begin{vmatrix} \left(\frac{1}{r} + \beta_1\right) & 0 & 0 \\ -\beta_1 & \left(\frac{1}{r} + \beta_2\right) & 0 \\ 0 & \beta_2 & \frac{1}{r} \end{vmatrix}}, \begin{vmatrix} \left(\frac{1}{r} + \beta_1\right) & 0 & 0 \\ -\beta_1 & \left(\frac{1}{r} + \beta_2\right) & 0 \\ 0 & \beta_2 & \frac{1}{r} \end{vmatrix} \neq 0$$

$$\Rightarrow \mathcal{A}\{\theta_2\} = \left(\frac{\omega\beta_1}{\beta_2-\beta_1}\right) \left[\frac{r^3}{1+\beta_1 r} - \frac{r^3}{1+\beta_2 r}\right] \quad (13)$$

$$\mathcal{A}\{\theta_3\} = \frac{\begin{vmatrix} \left(\frac{1}{r} + \beta_1\right) & 0 & r^2\omega \\ -\beta_1 & \left(\frac{1}{r} + \beta_2\right) & 0 \\ 0 & \beta_2 & 0 \end{vmatrix}}{\begin{vmatrix} \left(\frac{1}{r} + \beta_1\right) & 0 & 0 \\ -\beta_1 & \left(\frac{1}{r} + \beta_2\right) & 0 \\ 0 & \beta_2 & \frac{1}{r} \end{vmatrix}}, \begin{vmatrix} \left(\frac{1}{r} + \beta_1\right) & 0 & 0 \\ -\beta_1 & \left(\frac{1}{r} + \beta_2\right) & 0 \\ 0 & \beta_2 & \frac{1}{r} \end{vmatrix} \neq 0$$

$$\Rightarrow \mathcal{A}\{\theta_3\} = \omega \left[r^3 - \left(\frac{\beta_2}{\beta_2-\beta_1}\right) \left(\frac{r^3}{1+\beta_1 r}\right) + \left(\frac{\beta_1}{\beta_2-\beta_1}\right) \left(\frac{r^3}{1+\beta_2 r}\right) \right] \quad (14)$$

Performing inverse Anuj transform on equations (12), (13) and (14) gives the required concentrations $\theta_1(t)$, $\theta_2(t)$ and $\theta_3(t)$ as:

$$\begin{aligned} \theta_1 &= \mathcal{A}^{-1} \left\{ \frac{\omega r^3}{1+\beta_1 r} \right\} \\ \Rightarrow \theta_1 &= \omega \mathcal{A}^{-1} \left\{ \frac{r^3}{1+\beta_1 r} \right\} = \omega e^{-\beta_1 t} \end{aligned} \quad (15)$$

$$\begin{aligned} \theta_2 &= \mathcal{A}^{-1} \left\{ \left(\frac{\omega\beta_1}{\beta_2-\beta_1}\right) \left[\frac{r^3}{1+\beta_1 r} - \frac{r^3}{1+\beta_2 r}\right] \right\} \\ \Rightarrow \theta_2 &= \left(\frac{\omega\beta_1}{\beta_2-\beta_1}\right) \left[\mathcal{A}^{-1} \left\{ \frac{r^3}{1+\beta_1 r} \right\} - \mathcal{A}^{-1} \left\{ \frac{r^3}{1+\beta_2 r} \right\} \right] \\ \Rightarrow \theta_2 &= \left(\frac{\omega\beta_1}{\beta_2-\beta_1}\right) [e^{-\beta_1 t} - e^{-\beta_2 t}] \end{aligned} \quad (16)$$

$$\begin{aligned} \theta_3 &= \mathcal{A}^{-1} \left\{ \omega \left[r^3 - \left(\frac{\beta_2}{\beta_2-\beta_1}\right) \left(\frac{r^3}{1+\beta_1 r}\right) + \left(\frac{\beta_1}{\beta_2-\beta_1}\right) \left(\frac{r^3}{1+\beta_2 r}\right) \right] \right\} \\ \Rightarrow \theta_3 &= \omega \left[\mathcal{A}^{-1} \{r^3\} - \left(\frac{\beta_2}{\beta_2-\beta_1}\right) \mathcal{A}^{-1} \left\{ \frac{r^3}{1+\beta_1 r} \right\} + \left(\frac{\beta_1}{\beta_2-\beta_1}\right) \mathcal{A}^{-1} \left\{ \frac{r^3}{1+\beta_2 r} \right\} \right] \\ \Rightarrow \theta_3 &= \omega \left[1 - \left(\frac{\beta_2}{\beta_2-\beta_1}\right) e^{-\beta_1 t} + \left(\frac{\beta_1}{\beta_2-\beta_1}\right) e^{-\beta_2 t} \right] \end{aligned} \quad (17)$$

Remark 3: Results given by equations (15), (16) and (17) have perfect agreement with [36].

9. CONCLUSIONS: In this manuscript, we have profitably attained the solution of the problem of concentrations of the reactants of first order consecutive chemical reaction by using Anuj transform. It is observed that Anuj transform provide the exact analytical primitive of this problem with good accuracy. We can use Anuj transform to study the problems of chemical engineering in future that involve different order reversible and parallel chemical reactions.

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